$\mathcal{PT}$ symmetry as a necessary and sufficient condition for unitary time evolution

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Abstract

While Hermiticity of a time-independent Hamiltonian leads to unitary time evolution, in and of itself, the requirement of Hermiticity is only sufficient for unitary time evolution. Here we provide conditions that are both necessary and sufficient. Specifically, we show that $\mathcal{PT}$ symmetry of a time-independent Hamiltonian, or equivalently, reality of the secular equation that determines its eigenvalues, is both necessary and sufficient for unitary time evolution. For any $\mathcal{PT}$-symmetric Hamiltonian H there always exists an operator V that relates H to its Hermitian adjoint according to $VHV^{-1} = H^{\dagger}$. Hilbert space norms $\langle\psi_1|V|\psi_2\rangle$ constructed with this V are always preserved in time. With the energy eigenvalues of a real secular equation either being real or appearing in complex conjugate pairs, we thus establish the unitarity of time evolution for both stationary and non-stationary systems. In addition, we show that such systems obey causality.

I. UNITARY TIME EVOLUTION FOR NON-HERMITIAN HAMILTONIANS

If for a time-independent Hamiltonian H one constructs a time evolution operator of the form $U(t) = e^{-iHt}$, then if H is Hermitian, the adjoint operator $U^\dagger(t)$ is given by $U^\dagger(t) = e^{iHt}$ and the unitarity of $U(t)$ immediately follows. Moreover, if one introduces right-eigenvectors of H that obey

$$i\frac{d}{dt}|R_i(t)\rangle = H|R_i(t)\rangle, \tag{1}$$

then for Hermitian Hamiltonians the Dirac norm $\langle R_i(t)|R_i(t)\rangle$ is immediately preserved in time. However, if the Hamiltonian is not Hermitian, conjugation of (1) leads to

$$-i\frac{d}{dt}\langle R_i(t)| = \langle R_i(t)|H^\dagger, \tag{2}$$

with $U^\dagger(t)$ now being given by $U^\dagger(t) = e^{iH^\dagger t}$, and with the Dirac norm then not being time independent. Despite this, one cannot conclude that the time evolution associated with a non-Hermitian Hamiltonian is not unitary. Rather, all one can conclude is that the standard derivation of unitarity for Hermitian Hamiltonians and the appropriateness of the Dirac norm do not apply when the Hamiltonian is not Hermitian. While the above analysis shows that Hermiticity implies unitarity, one cannot conclude that lack of Hermiticity implies lack of unitarity. And indeed, a whole class of non-Hermitian Hamiltonians has been identified in which time evolution is unitary, namely those in which the Hamiltonian possesses a $\mathcal{PT}$ symmetry and has a set of energy eigenvalues that are all real (see the review of [1] and references therein). The purpose of this paper is to identify all possible classes of Hamiltonians for which time evolution is unitary, with Hermitian Hamiltonians being just one of the possible classes.

The key to finding the general rule is to recognize that if $|R_i(t)\rangle$ is an eigenstate of H with some general complex energy $E_i = E_i^R + iE_i^I$, then on introducing some general time-independent operator V, the V-dependent inner product $\langle R_j(t)|V|R_i(t)\rangle$ will be given by

$$\langle R_j(t)|V|R_i(t)\rangle = e^{-i(E_i^R - E_j^R)t + (E_i^I + E_j^I)t}\langle R_j(t=0)|V|R_i(t=0)\rangle. \tag{3}$$

This inner product will be time independent for energies that obey the two conditions

$$E_i^R - E_j^R = 0, \qquad E_i^I + E_j^I = 0, \tag{4}$$

and will be time independent for states with energies that do not obey these conditions if an operator V can be found so that for all of those states the matrix element $\langle R_j(t =$

$0)|V|R_i(t=0)\rangle$ vanishes. The eigenstates of Hermitian Hamiltonians immediately obey these conditions with $E_i^I = 0$, $E_j^I = 0$ and $V = I$. However in the general case one needs a non-trivial V, and a thus non-Dirac norm.

To find the general conditions under which the needed V will in fact exist, we note that from (1) and (2) we can evaluate the time derivative of $\langle R_j(t)|V|R_i(t)\rangle$ to obtain

$$i\frac{d}{dt}\langle R_j(t)|V|R_i(t)\rangle = \langle R_j(t)|(VH - H^\dagger V)|R_i(t)\rangle. \tag{5}$$

Thus if, just as is needed to establish unitarity for Hermitian Hamiltonians, we require that the set of states $|R_i(t)\rangle$ be complete for the general H, we see that all matrix elements $\langle R_j(t)|V|R_i(t)\rangle$ will be time independent if V obeys the relation

$$VHV^{-1} = H^\dagger \tag{6}$$

as an operator identity. The needed V is thus the one that effects the transformation from H to its Hermitian adjoint $H^\dagger$. Conversely, if a Hamiltonian has the property that H and $H^\dagger$ can be related by an operator V as in (6), it follows from (5) that all matrix elements $\langle R_j(t)|V|R_i(t)\rangle$ constructed with this V are time independent. The condition that there exist an operator V that effects $VHV^{-1} = H^\dagger$ is thus a necessary and sufficient condition for unitary time evolution. We note that as defined in (6) the operator V depends on the Hamiltonian. Thus unlike the standard Dirac norm $\langle R_j(t)|R_i(t)\rangle$, the $\langle R_j(t)|V|R_i(t)\rangle$ norm cannot be preassigned, with it being dynamically determined by the Hamiltonian itself.

When there does exist an operator V for which (6) is satisfied, we can rewrite (2) as

$$-i\frac{d}{dt}\langle R_i(t)|V = \langle R_i(t)|VH. \tag{7}$$

In such a situation the state $\langle L_i(t)| = \langle R_i(t)|V$ is a left-eigenvector of H as it obeys

$$-i\frac{d}{dt}\langle L_i(t)| = \langle L_i(t)|H, \tag{8}$$

with unitary time evolution thus being associated with Hamiltonians that have complete sets of both left- and right-eigenvectors. In terms of the left-eigenvectors the $\langle R_j(t)|V|R_i(t)\rangle$ inner product can be written as $\langle L_j(t)|R_i(t)\rangle$, with the inner product thus being the overlap of the left- and right-eigenvectors of the Hamiltonian, an overlap that is manifestly time independent because of (1) and (8). The general rule then is to define the inner product as the overlap of the left- and right-eigenvectors, and so we need to ascertain the conditions on H for which a V operator that satisfies (6) (and thus the left-eigenvectors that it then generates) will necessarily exist.

II. $\mathcal{PT}$ SYMMETRY AND THE $VHV^{-1} = H^\dagger$ CONDITION

When H and $H^\dagger$ are related according to the similarity transform $VHV^{-1} = H^\dagger$, the determinant condition for the eigenvalues of H obeys $\det(H - \lambda I) = \det(V^{-1}H^\dagger V - \lambda I) = \det(H^\dagger - \lambda I) = \det((H^*)^{\rm TR} - \lambda I) = \det(H^* - \lambda I) = 0$, where TR denotes transpose. Consequently, H and H^* possess the same set of eigenvalues, with the secular equation $\det(H - \lambda I) = 0$ thus being real. With the energies of a real secular equation either being real or appearing in complex conjugate pairs, one can immediately satisfy (4) non-trivially, just as required. Conversely, if the secular equation that determines the energy eigenvalues is real, then H and $H^\dagger$ will possess the same set of eigenvalues and thus be related by an isospectral similarity transform. Reality of the secular equation is thus both necessary and sufficient for the existence of a V operator that obeys (6). Reality of the secular equation is thus both necessary and sufficient for unitary time evolution.

The reality requirement on a secular equation is a condition that is encountered in $\mathcal{PT}$-symmetric theories ($\mathcal{P}$ and $\mathcal{T}$ denote parity and time reversal). Specifically, it was noted in [2] that if a Hamiltonian is $\mathcal{PT}$ symmetric, the secular equation would be real. Moreover, it is not specifically $\mathcal{PT}$ invariance itself that is required for the proof. All one needs is that H be invariant under the action of the product of a discrete linear operator and a discrete anti-linear operator. For a time-independent H, time reversal reduces to complex conjugation K times a matrix that acts in the space of the eigenvectors of H, with $\mathcal{PT}$ then acting as AK where A is a matrix. The essence of the proof of the reality of the secular equation is to note that if a Hamiltonian commutes with AK, the determinant condition then obeys $\det(H - \lambda I) = \det(AKHKA^{-1} - \lambda I) = \det(KHK - \lambda I) = \det(H^* - \lambda I) = 0$, with reality of the secular equation immediately following. Discussion of the reality of secular equations dates back to Wigner [3], who considered invariance of a Hamiltonian under time reversal alone. Modern interest in the reality of secular equations was triggered by the surprising discovery that the non-Hermitian Hamiltonian $H = p^2/2m + ix^3$ had a completely real eigenspectrum [4, 5], an outcome that was traced in [5] to the fact that while not time reversal invariant, H was nonetheless invariant under the $\mathcal{PT}$ product as $\mathcal{T}$ transforms i into $-i$ while $\mathcal{P}$ transforms x into $-x$. The utility of $\mathcal{PT}$ invariance stems from the fact that complex potentials that are not $\mathcal{T}$ invariant might still be invariant with respect to a $\mathcal{PT}$ product where $\mathcal{P}$ is an appropriate linear operator, and thus yield a real secular equation.

In [2] it was shown that if a Hamiltonian is $\mathcal{PT}$ symmetric then its secular equation is real. More recently, the converse has been proven [6], namely that if a Hamiltonian has a secular equation that is real, then one can always find appropriate $\mathcal{P}$ and $\mathcal{T}$ operators under which the Hamiltonian is $\mathcal{PT}$ symmetric. Consequently, $\mathcal{PT}$ symmetry of a Hamiltonian is both necessary and sufficient for reality of its secular equation, and thus $\mathcal{PT}$ symmetry of a Hamiltonian is both necessary and sufficient for unitary time evolution. The power of this result is that one can determine whether or not a Hamiltonian can generate unitary time evolution entirely by examining its symmetry structure under the action of the product of a discrete linear operator and a discrete anti-linear operator.

Within the family of Hamiltonians that have real secular equations there are three cases of interest: (i) the energies are all real and the energy eigenvectors are complete, (ii) the energy eigenvectors are complete but the energies include one or more complex conjugate pairs, and (iii) the energies are real but the energy eigenvectors do not form a complete set and the Hamiltonian is in non-diagonalizable, Jordan block form. A possible fourth case, namely that the energy eigenvectors are not complete and the energies include one or more complex conjugate pairs, is not allowed since the energies of a Jordan-block matrix are all equal (they all share a single common eigenvector) and could thus not contain any complex conjugate pairs [6]. Moreover, in [6] criteria were also provided for determining to which of these three cases of interest any given $\mathcal{PT}$-symmetric Hamiltonian belongs. Specifically, in the general analysis of $\mathcal{PT}$-symmetric Hamiltonians it has been found to be very convenient [1] to introduce a linear operator, the $\mathcal{C}$ operator, that obeys the two conditions: $[\mathcal{C}, H] = 0$, $\mathcal{C}^2 = 1$. In [6] it was shown that if every $\mathcal{C}$ that non-trivially obeys these two conditions commutes with $\mathcal{PT}$ then we are in case (i), that if there exists at least one $\mathcal{C}$ that does not commute with $\mathcal{PT}$ then we are in case (ii), and if there is no $\mathcal{C}$ that obeys these two conditions at all then we are in case (iii). Thus as well as ascertain the unitarity structure of a Hamiltonian via a symmetry condition (i.e. whether or not H commutes with $\mathcal{PT}$), we can even determine which realization of the energy spectrum we are in by examining the structure of a commutator (viz. that of $\mathcal{C}$ with $\mathcal{PT}$). We now examine how the unitarity of time evolution works in each of these three cases in detail.

III. UNITARITY WHEN ENERGIES ARE ALL REAL AND COMPLETE

For the case of a $\mathcal{PT}$-invariant Hamiltonian whose energy spectrum is both real and complete, it can be shown [1, 6, 7] that the operator V can always be written as e^{-Q} where Q is a Hermitian operator, and that the operator e^{-Q} itself can always be written as $e^{-Q} = P\mathcal{C}$ where $\mathcal{C}$ is the $\mathcal{C}$ operator discussed above. The utility of the Q operator is that its Hermiticity ensures that the operator $\tilde{H} = e^{-Q/2} H e^{Q/2}$ is Hermitian [1, 8]. If for $\tilde{H}$ we introduce a standard set of right-eigenstates $|\tilde{n}^i\rangle$, the right-eigenstates of H are thus related to those of $\tilde{H}$ by the mapping $|n_i\rangle = e^{Q/2}|\tilde{n}_i\rangle$. Since Q is Hermitian and $e^{-Q/2}$ is a similarity transform but not a unitary one, the states $\langle n_i| = \langle \tilde{n}_i| e^{Q/2}$ are not left-eigenstates of H. Rather, it is the states $\langle n_i| e^{-Q}$ that are the left-eigenstates. Moreover, since the eigenstates of the Hermitian $\tilde{H}$ obey the standard time-independent Dirac orthonormality condition $\langle \tilde{n}^i | \tilde{n}^j \rangle = \delta_{i,j}$, then by the mapping the eigenstates of H obey the time-independent condition $\langle n^i | e^{-Q} | n^j \rangle = \delta_{i,j}$. With $V = e^{-Q}$, we recognize the inner product $\langle n^i | e^{-Q} | n^j \rangle$ as being none other than the time-independent V-operator norm introduced above [9].

The essence of the above analysis is the realization that when a Hamiltonian H has an energy spectrum that is both real and complete, the Hamiltonian is either already Hermitian or can be brought to a Hermitian form $\tilde{H}$ by a similarity transformation. However, if a Hamiltonian H is not Hermitian the needed similarity transformation will not be unitary and the basis states of H will not be orthonormal with respect to the Dirac inner product. Rather, they will form a skew basis, with it being the similarity transform that puts the basis into an orthonormal form. $\mathcal{PT}$-symmetric Hamiltonians that are not Hermitian but nonetheless have a real and complete eigenspectrum are thus Hermitian in disguise. Consequently, they are unitary in disguise too, with it being the V-operator norm that is the appropriate norm for the Hamiltonian.

It is instructive to recast the above discussion in the language of the S-matrix. For the above $|\tilde{n}_i\rangle$ basis first, we can define complete sets of in and out states that obey the standard closure relations $\sum_i |\tilde{n}^i_{in}\rangle\langle\tilde{n}^i_{in}| = I$ and $\sum_i |\tilde{n}^i_{out}\rangle\langle\tilde{n}^i_{out}| = I$. Given these relations one can show that the scattering operator defined by $\tilde{S} = \sum_i |\tilde{n}^i_{in}\rangle\langle\tilde{n}^i_{out}|$ and thus by $\tilde{S}^\dagger = \sum_i |\tilde{n}^i_{out}\rangle\langle\tilde{n}^i_{in}|$ immediately obeys the unitarity relation $\tilde{S}\tilde{S}^\dagger = I$.

Since the in and out states of $\tilde{H}$ can be mapped into the in and out states of H by the mapping, an S-matrix operator in the $|n_i\rangle$ basis can thus be defined via the mapping as

$\tilde{S} = e^{-Q/2} S e^{Q/2}$, with the adjoint $S^\dagger$ being given via $\tilde{S}^\dagger = e^{Q/2} S^\dagger e^{-Q/2}$ since the operator Q is Hermitian. As constructed, the operator S can be written as $S = e^{Q/2} \sum_i |\tilde{n}^i_{in}\rangle\langle\tilde{n}^i_{out}| e^{-Q/2}$, and from the mapping thus takes the form $S = \sum_i |n^i_{in}\rangle\langle n^i_{out}| e^{-Q}$ in the $|n_i\rangle$ basis. In addition, the $\tilde{S}\tilde{S}^\dagger = I$ relation obliges S to obey $e^{-Q/2} S e^{Q/2} e^{Q/2} S^\dagger e^{-Q/2} = I$, i.e. to obey

$$S e^{Q} S^\dagger e^{-Q} = I, \qquad e^{-Q} S e^{Q} S^\dagger = I. \tag{9}$$

It is thus (9) that is the form that unitarity of a scattering process takes in a skew basis.

While we have derived (9) by transforming to the Hermitian basis and then transforming back, it is possible to derive (9) directly in the $|n_i\rangle$ basis without needing to make any reference to the tilde basis at all. Moreover, there is a more general derivation that does not even require us to restrict to Hermitian V. Specifically, we note that for energy eigenstates, be they real or complex, the time independence of $\langle R_j(t)|V|R_i(t)\rangle$ as required by (5) and (6) entails that states whose energies do not obey (4) have to obey $\langle R_j(t=0)|V|R_i(t=0)\rangle = 0$. Consequently, such states are orthogonal with respect to the V-operator norm, and on normalizing the states appropriately, for all energy eigenstates we can thus set $\langle R_j(t)|V|R_i(t)\rangle = \delta_{i,j}$. With this orthonormality relation we obtain orthonormality and closure relations for the in and out states of the form

$$\begin{aligned}
&\langle n^i_{in}|V|n^j_{in}\rangle = \langle n^j_{in}|V^\dagger|n^i_{in}\rangle = \delta_{i,j}, \qquad \langle n^i_{out}|V|n^j_{out}\rangle = \langle n^j_{out}|V^\dagger|n^i_{out}\rangle = \delta_{i,j}, \\
&\sum_i |n^i_{in}\rangle\langle n^i_{in}|V = \sum_i V^\dagger|n^i_{in}\rangle\langle n^i_{in}| = I, \quad \sum_i |n^i_{out}\rangle\langle n^i_{out}|V = \sum_i V^\dagger|n^i_{out}\rangle\langle n^i_{out}| = I.
\end{aligned} \tag{10}$$

If we now define an operator $S = \sum_i |n^i_{in}\rangle\langle n^i_{out}|V$, from (10) we obtain

$$S V^{-1} S^\dagger V = \sum_i |n^i_{in}\rangle\langle n^i_{out}| V V^{-1} \sum_j V^\dagger |n^j_{out}\rangle\langle n^j_{in}| V = \sum_i |n^i_{in}\rangle\langle n^i_{in}| V = I. \tag{11}$$

Consequently, for PT-invariant Hamiltonians unitarity of the scattering process thus takes the equivalent forms

$$S V^{-1} S^\dagger V = I, \qquad V S V^{-1} S^\dagger = I. \tag{12}$$

As a simple check on (12), we note that if S is written as the evolution operator $S = e^{-iHt}$, then because $H^\dagger = V H V^{-1}$, it follows that $V S V^{-1}$ is given as $e^{-iH^\dagger t}$. Then with $S^\dagger = e^{+iH^\dagger t}$, (12) immediately follows. The relation given in (12) is thus the unitarity relation we want. While we shall discuss the complex energy case in more detail below, as we had already noted, our derivation of (12) holds even if some energies are complex. The issue here is

not whether or not we can prepare stable in and out states with them, but whether or not we need them for the closure relations given in (10). In other words, suppose we have a PT-invariant Hamiltonian with N real energy eigenvalues and M complex pairs. For such a situation, unitarity in the form given in (12) will only follow if in the closure relations in (10) we sum over $N+2M$ states (i.e. over $N+2M$ channels), and not over N states alone.

As well as provide a formal derivation of our results, it is instructive to see how our ideas work in a simple model. Since we can always diagonalize any Hamiltonian that possesses a complete set of eigenstates, and since complex congugate pairs would form a two-dimensional subblock in the diagonal basis, it will suffice to discuss a two-dimensional model. We thus follow [1] and introduce the Hamiltonian (the parameters r, s and θ are real)

$$H = r\cos\theta\sigma_0 + ir\sin\theta\sigma_3 + s\sigma_1 = \begin{pmatrix} r\cos\theta + ir\sin\theta & s \\ s & r\cos\theta - ir\sin\theta \end{pmatrix}. \qquad (13)$$

While not Hermitian, this H is $\mathcal{PT}$ invariant under $\mathcal{P} = \sigma_1$, $\mathcal{T} = K$ and thus has a real secular equation with energies being given by $E_\pm = r\cos\theta \pm (s^2 - r^2\sin^2\theta)^{1/2}$. In the region where $s^2 - r^2\sin^2\theta$ is positive the two energy eigenvalues are real and distinct. In this region we can define a Hermitian operator $e^{-Q/2}$ according to

$$e^{\mp Q/2} = \left(\frac{1+\sin\alpha}{2\sin\alpha}\right)^{1/2}\sigma_0 \pm \sigma_2\left(\frac{1-\sin\alpha}{2\sin\alpha}\right)^{1/2}, \qquad e^{\mp Q} = \frac{1}{\sin\alpha}\sigma_0 \pm \sigma_2\frac{\cos\alpha}{\sin\alpha}, \qquad (14)$$

where $\sin\alpha = +(s^2 - r^2\sin^2\theta)^{1/2}/s$, $\cos\alpha = r\sin\theta/s$. Using the $e^{-Q/2}$ operator we construct

$$\tilde{H} = e^{-Q/2}He^{Q/2} = r\cos\theta\sigma_0 + \sigma_1(s^2 - r^2\sin^2\theta)^{1/2}, \qquad (15)$$

and confirm that $\tilde{H}$ is Hermitian when $s^2 - r^2\sin^2\theta$ is positive. Similarly we construct $e^{-Q}He^{Q}$ and confirm that it is equal to $H^\dagger$. Finally, we construct an operator $C = e^Q P$, viz.

$$C = \frac{1}{\sin\alpha}\left(\sigma_1 + i\cos\alpha\sigma_3\right), \qquad (16)$$

and confirm that it not only obeys $[\mathcal{C}, H] = 0$ and $\mathcal{C}^2 = I$, it also obeys $[\mathcal{C}, \mathcal{PT}] = 0$, just as it must since the energies are real.

In the region where $s^2 - r^2\sin^2\theta$ is positive, eigenvector solutions that obey $idu_\pm/dt = Hu_\pm = E_\pm u_\pm$ are given as

$$u_+ = \frac{e^{-i(r\cos\theta+\mu)t}e^{i\pi/4}}{(2\sin\alpha)^{1/2}}\begin{pmatrix} e^{-i\alpha/2} \\ -ie^{i\alpha/2} \end{pmatrix}, \qquad u_- = \frac{e^{-i(r\cos\theta-\mu)t}e^{i\pi/4}}{(2\sin\alpha)^{1/2}}\begin{pmatrix} ie^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix}. \qquad (17)$$

where $\mu = +(s^2 - r^2 \sin^2\theta)^{1/2}$. For the states in (17) the e^{-Q} norms obey the time-independent and manifestly unitary orthonormality and closure relations

$$u_\pm^\dagger e^{-Q} u_\pm = +1, \qquad u_\pm^\dagger e^{-Q} u_\mp = 0, \qquad u_+ u_+^\dagger e^{-Q} + u_- u_-^\dagger e^{-Q} = I, \tag{18}$$

just as required. It is thus the $V = e^{-Q}$ norm that it is the appropriate one for the problem.

IV. UNITARITY WHEN ENERGIES ARE NOT ALL REAL BUT COMPLETE

To determine what happens when energies are complex, it is instructive to study the two-dimensional model in the regime where $s^2 - r^2 \sin^2\theta$ is negative. Now the energies are given by the complex conjugate pair $E_\pm = r\cos\theta \pm i\nu$ where $\nu = +(r^2 \sin^2\theta - s^2)^{1/2}$. In this region we can define a now non-Hermitian operator $e^{-Q/2}$ according to

$$e^{\mp Q/2} = \left(\frac{1 + i\sinh\beta}{2i\sinh\beta}\right)^{1/2} \sigma_0 \pm \sigma_2 \left(\frac{1 - i\sinh\beta}{2i\sinh\beta}\right)^{1/2}, \qquad e^{\mp Q} = \frac{1}{i\sinh\beta}\sigma_0 \pm \sigma_2 \frac{\cosh\beta}{i\sinh\beta}, \tag{19}$$

where $\sinh\beta = +(r^2\sin^2\theta - s^2)^{1/2}/s$, $\cosh\beta = r\sin\theta/s$. Using this $e^{-Q/2}$ operator we construct

$$\tilde{H} = e^{-Q/2} H e^{Q/2} = r\cos\theta\sigma_0 + i\sigma_1 (r^2\sin^2\theta - s^2)^{1/2}, \tag{20}$$

and see that $\tilde{H}$ is not Hermitian when $s^2 - r^2\sin^2\theta$ is negative. Despite this, we construct $e^{-Q} H e^{Q}$ with this non-Hermitian Q and confirm that it nonetheless is equal to $H^\dagger$, just as it must be. Finally, we construct an operator $C = e^Q P$, viz.

$$C = \frac{1}{i\sinh\beta}\left(\sigma_1 + i\cosh\beta\sigma_3\right) \tag{21}$$

and confirm that it while it obeys $[\mathcal{C}, H] = 0$ and $\mathcal{C}^2 = I$, because of its overall factor of i it does not obey $[\mathcal{C}, \mathcal{PT}] = 0$, as must be the case since the energies are not real.

In the region where $s^2 - r^2\sin^2\theta$ is negative, eigenvector solutions that obey $i du_\pm/dt = H u_\pm = E_\pm u_\pm$ can be constructed by setting $\mu = i\nu$, $\alpha = i\beta$ in (17), and are given as

$$u_+ = \frac{e^{-ir\cos\theta t + \nu t}}{(2\sinh\beta)^{1/2}} \begin{pmatrix} e^{\beta/2} \\ -ie^{-\beta/2} \end{pmatrix}, \quad u_- = \frac{e^{-ir\cos\theta t - \nu t}}{(2\sinh\beta)^{1/2}} \begin{pmatrix} ie^{-\beta/2} \\ e^{\beta/2} \end{pmatrix}. \tag{22}$$

For the states in (22) the e^{-Q} norms obey the time-independent orthogonality and closure relations

$$\begin{aligned} &u_\pm^\dagger e^{-Q} u_\pm = 0, \qquad u_-^\dagger e^{-Q} u_+ = +1, \qquad u_+^\dagger e^{-Q} u_- = -1, \\ &u_+ u_-^\dagger e^{-Q} - u_- u_+^\dagger e^{-Q} = I. \end{aligned} \tag{23}$$

With the adjoints of the states in (22) having time dependences of the form $u_+^\dagger \sim e^{ir\cos\theta t+\nu t}$, $u_-^\dagger \sim e^{ir\cos\theta t-\nu t}$, we see that in (23) those overlaps that are zero have to vanish through the e^{-Q} matrix structure of the overlaps since the time dependences in $u_\pm^\dagger e^{-Q}u_\pm$ do not cancel each other once ν is non-zero. For the non-zero overlaps the time dependences in $u_\mp^\dagger e^{-Q}u_\pm$ do precisely cancel each other, just as required by (4). With the u_+ and u_- states in (22) obeying $\mathcal{PT}u_+ = u_-$, $\mathcal{PT}u_- = u_+$ ($\mathcal{T}$ effects $t \to -t$ as well as $i \to -i$), the non-vanishing overlaps in (23) represent transitions between energy eigenstates and their $\mathcal{PT}$ partners [10].

The most notable aspect of the overlaps is that the $u_+^\dagger e^{-Q}u_-$ overlap is negative. However, this does not herald the presence of a negative metric since the overlap is a transition matrix element between different states and not the overlap of a state with its own adjoint. Moreover, rather than being an indicator of a possible loss of unitarity, this negative sign is actually needed for unitarity. Specifically, if we construct a propagator $D(E)$ for above Hamiltonian, it will have the form of matrix elements of the states divided by energy denominators:

$$D(E) = \frac{u_-^\dagger e^{-Q}u_+}{E-(E_R+iE_I)} + \frac{u_+^\dagger e^{-Q}u_-}{E-(E_R-iE_I)}, \tag{24}$$

and thus evaluate to

$$D(E) = \frac{1}{E-(E_R+iE_I)} - \frac{1}{E-(E_R-iE_I)} = \frac{2iE_I}{(E-E_R)^2+E_I^2}. \tag{25}$$

Other than the overall factor of 2, the imaginary part of this propagator is the same as that of a standard Breit-Wigner

$$D_{\rm BW}(E) = \frac{1}{E-(E_R+iE_I)} = \frac{E-E_R+iE_I}{(E-E_R)^2+E_I^2}. \tag{26}$$

The negative sign of $u_+^\dagger e^{-Q}u_-$ thus compensates for the negative sign of the imaginary part of the energy of the u_- state, with its contribution to the imaginary part of $D(E)$ then being positive rather than negative [11].

While it is nice to see that $D(E)$ recovers the standard Breit-Wigner form, our results actually go further than that as they provide some justification for the use of the standard $D_{\rm BW}(E)$ in the first place. Specifically, if one works with a general complex potential, i.e. with one for which (4) is not obeyed, one would not get unitary time evolution. If for instance we work with a complex potential that has just one energy eigenstate with wave function $\psi = e^{-iE_Rt+E_It}$, the probability would be given as $\psi^*\psi = e^{-2E_It}$ and not be preserved in time, and would even grow in time if E_I is negative. Hence, if we wish to describe absorption or

decay processes in a time-preserving manner, we must augment this state with its complex conjugate partner and include the contribution of the partner to $D(E)$. Our approach is thus well-suited to a scattering process in which the in and out states long before and long after a collision are real eigenvalue eigenstates of a $\mathcal{PT}$-invariant Hamiltonian H_0, with the states scattering through some short-range $\mathcal{PT}$-invariant interaction $H_{\rm INT}$ for which $H_0 + H_{\rm INT}$ has complex eigenvalues. In such a situation the interaction would generate two poles at $E_R \pm iE_I$ that would be on the same Riemann sheet and combine just as in (25) [12].

The fact that the two complex conjugate poles are on the same Riemann sheet has an interesting consequence: it enables the two poles to be located within the same contour in the complex energy plane rather than be in different contours. In consequence, the theory will be causal. Specifically, with two complex conjugate poles having opposite imaginary parts, one of the poles would have to appear above the real energy axis and one below. Now when one only has to deal with poles with real energies (such as the $D(E) = 1/E_+ + 1/E_-$ propagator associated with (18)), to construct a causal, retarded propagator, one locates all the poles slightly below the real axis, with a contour integration then giving no pole contribution if one closes the contour in the upper-half plane. If one simply repeats this prescription when there is a pole in the upper-half plane, on closing the contour above the real axis one then gets a non-zero pole contribution and causality violations result. However, as discussed for instance in [13], for complex conjugate pairs of poles one can use an alternate contour instead. Specifically, one can deform the contour to pass above any pole in the upper-half plane. Then when one closes this deformed contour in the upper-half plane, one still gets no pole contribution and the propagator is causal, and when one closes the deformed contour in the lower-half plane, both complex poles contribute, just as in (25). For $\mathcal{PT}$ theories then, to maintain causality, the prescription is to make the choice of contour dynamics dependent (just as is done with the $\mathcal{PT}$-theory Hilbert space metric), so that as interactions cause poles to move off the real axis the contour must move along with them so that all the poles remain below it, a meaningful procedure if all the poles are on the same Riemann sheet [14].

V. UNITARITY WHEN ENERGIES ALL REAL BUT INCOMPLETE

When a Hamiltonian is diagonalizable, one does not need to distinguish between the eigenvalue solutions to the secular equation $\det(H - \lambda I) = 0$ and the eigenvalue solutions

to $H\psi = E\psi$ since the two sets of solutions coincide. However, when a Hamiltonian is not diagonalizable, the number of eigensolutions to $H\psi = E\psi$ is less than the number of eigenvalue solutions to $\det(H - \lambda I) = 0$, and the spectrum of H is incomplete. A typical example of a non-diagonalizable, Jordan-block, matrix is the two-dimensional matrix M

$$M = \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix}. \tag{27}$$

Its secular equation $|M - \lambda I| = 0$ has two solutions for λ, both of which are equal to a (and incidentally both solutions are real when a is real even though an M with real a is not Hermitian), but M has only one right-eigenvector and equally only one left-eigenvector, viz.

$$\begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad a \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix}. \tag{28}$$

Despite the lack of completeness of its eigenstates, if the secular equation $\det(H - \lambda I) = 0$ of a Hamiltonian is real, H and its adjoint $H^\dagger$ will still be related by (6), i.e. still be related $VHV^{-1} = H^\dagger$ for some operator V. For the example of (28) the secular equation will be real when a is real, and V will then be given by $V = \sigma_1$ [15]. More generally, for a non-diagonalizable matrix of arbitrary dimensionality, Jordan showed that via a sequence of similarity transformations any such matrix can always be brought to the Jordan canonical form in which all of the elements on the diagonal are equal to each other, and the only non-zero off-diagonal elements are all real and all lie on the superdiagonal immediately above the diagonal. With the non-zero elements on the superdiagonal not contributing to the secular equation since all the other non-diagonal elements of the matrix are zero, the elements on the diagonal of a Jordan block matrix are the eigenvalue solutions to the secular equation. Since all the eigenvalues of a Jordan-block matrix have to be equal to each other, the reality of the secular equation of a Jordan-block matrix requires that all of its solutions be real, since any complex conjugate pair of solutions could not be equal to each other. Thus for any Jordan-block matrix whose secular equation is real, we see that all the elements of the matrix are real, with the Hermitian adjoint of the matrix thus being equal to its transpose. Since a transposition matrix always exists in any dimension (an explicit construction is given in [6]), the transposition matrix serves as V. Thus for any Jordan-block matrix with a real secular equation, one can always find an operator V that effects $VHV^{-1} = H^\dagger$.

Moreover, in the Jordan block case the converse also holds. Specifically if one can find a V operator that effects $VHV^{-1} = H^\dagger$, the secular equation will be real since the invariance

of a determinant under similarity transforms is insensitive to Jordan-block structures. Thus even in the Jordan block case $\mathcal{PT}$ invariance is necessary and sufficient for the existence of a V operator that effects $VHV^{-1} = H^\dagger$.

With (5) holding for any states that obey (1) and (2), (5) will hold for non-stationary as well as stationary solutions to (1). Now in the Jordan block case the lack of energy eigenstates is compensated for (see e.g. [16]) by the presence of non-stationary solutions that typically behave as powers of t. For every missing stationary solution one finds a power-behaved in t solution [17]. The set of all stationary plus non-stationary solutions combined is thus complete [18]. Since the stationary plus non-stationary solutions are complete, we can use (5) to infer that in the Jordan block case time evolution of wave packets will be unitary if and only if one can find a V operator that effects $VHV^{-1} = H^\dagger$. Thus, as noted in [16], even though the non-stationary solutions are power-behaved in t, packets containing them and the stationary solutions will still evolve with a probability that is preserved in time [19].

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[9] With $\mathcal{C}$ commuting with $\mathcal{PT}$ when all energies are real, we can take all the energy eigenstates to be eigenstates of $\mathcal{CPT}$ with eigenvalue one. With $\mathcal{C} = e^Q P$ and thus with $\mathcal{C}^\dagger = \mathcal{P}e^Q$ since $\mathcal{P}$ and Q are Hermitian, we can write the norm as $((\mathcal{CPT}u)^\dagger, e^{-Q}v) = (u^{\rm TR}, \mathcal{P}^\dagger\mathcal{P}v) = (u^{\rm TR}, v) =$

$((\mathcal{CPT}u)^{\rm TR}, v)$, to thus recover the $t = 0$ norm used in [1] for eigenstates with real energies.

[10] This transition structure also holds when all energy eigenvalues are real, with the states in (17) obeying $\mathcal{PT}u_\pm = \pm u_\pm$ (as well as $\mathcal{C}u_\pm = \pm u_\pm$, $\mathcal{CPT}u_\pm = u_\pm$), so that the non-zero overlaps are between states and themselves as they are their own $\mathcal{PT}$ partners. (This $\mathcal{PT}$ structure of energy eigenstates is generic, since, as noted in [1], for real energies the energy eigenstates are eigenstates of $\mathcal{PT}$, and for complex conjugate energies the energy eigenstates transform into each other under $\mathcal{PT}$.)

[11] A similar effect is observed in Lee-Wick electrodynamics (T. D. Lee and G. C. Wick, Nucl. Phys. B **9**, 209 (1969); **10**, 1 (1969); Phys. Rev. D **2**, 1033 (1970)) where a pair of states with complex conjugate energies combine as in (25) to produce a unitary propagator. The difference between the approach here and that of Lee and Wick is that Lee and Wick attributed the needed minus sign in (25) to an intrinsic property of the Hilbert space by employing a preassigned indefinite metric in which $u_-^\dagger u_-$ (the overlap of u_- with itself) is taken to be negative and the closure relation is of the generic, so-called Krein space, form $u_+u_+^\dagger - u_-u_-^\dagger = I$. In our work here we do not work with an indefinite metric, nor do we preassign the metric. Rather the e^{-Q} inner product is determined by the theory itself, with the e^{-Q} norm not being a universal norm but being one that depends each time on the particular form of the Hamiltonian, as it is defined as the operator that effects $e^{-Q}He^Q = H^\dagger$. In fact, in general the key difference between the norms needed for Hermitian and $\mathcal{PT}$ theories is that while the Hermitian case norm can be assigned a priori (c.f. the Dirac norm or its quasi-Hermitian negative metric Krein space generalization), for $\mathcal{PT}$ theories each Hamiltonian determines its own e^{-Q} norm. It was by taking advantage of this fact that Bender and Mannheim (C. M. Bender and P. D. Mannheim, Phys. Rev. Lett. **100**, 110402 (2008); J. Phys. A **41**, 304018 (2008): C. M. Bender and P. D. Mannheim, Phys. Rev. D **78**, 025022 (2008)) were able to show that theories based on the fourth-order propagator $D(k^2) = 1/k^2 - 1/(k^2 + M^2)$ were unitary theories that did not need to be formulated in an indefinite metric Hilbert space. (With the poles of this fourth-order propagator being both real and complete, the associated Hilbert space closure relation is of the generic form $u_+u_+^\dagger e^{-Q} + u_-u_-^\dagger e^{-Q} = I$ given in (18), with the relative minus sign in the fourth-order propagator being associated with a negative eigenvalue of the $e^{-Q} = PC$ operator.) Moreover, by establishing that the fourth-order derivative conformal gravity theory is a $\mathcal{PT}$ theory, conformal gravity is now able to emerge as a fully

consistent, renormalizable, and unitary theory of quantum gravity in four spacetime dimensions (P. D. Mannheim, *Comprehensive Solution to the Cosmological Constant, Zero-Point Energy, and Quantum Gravity Problems*, arXiv:0909.0212v3 [hep-th], September 2009).

[12] It would be of interest to see if the factor of 2 in (25) might lead to some observable consequence, perhaps in the determination of branching ratios.

[13] S. Coleman, *Acausality*, in Subnuclear Phenomena: International School of Physics Ettore Majorana, Erice, Italy, 1969, A. Zichichi (Ed.), Academic Press, New York (1970).

[14] It could be of interest to see if the causality problems that are met in Lee-Wick electrodynamics [11, 13] might originate in the use of a preassigned Krein space norm rather than the dynamically determined e^{-Q} norm.

[15] For the 2-dimensional example given in (13), when we let α go to zero the two eigenvalues E_+ and E_- both become become equal to $r\cos\theta$, and the two eigenvectors u_+ and u_- in (17) collapse onto a single eigenvector, with the Hamiltonian becoming Jordan block in the limit. At the point where α becomes zero, both e^{-Q} and $\mathcal{C}$ become undefined, just as they must because $\alpha = 0$ is the transition point between the phase where the energies are real and the phase where they are complex. Despite this, H and $H^\dagger$ themselves (as well as $\mathcal{P}$ and $\mathcal{T}$) remain well-defined when $\alpha \to 0$ since one just sets $s = r\sin\theta$ in H. Despite the fact that both e^{-Q} and e^{Q} become undefined in the limit, the product $e^{-Q}He^{Q}$ remains well-defined, and thus continues to be equal to $H^\dagger$.

[16] C. M. Bender and P. D. Mannheim, Phys. Rev. D **78**, 025022 (2008)).

[17] As the parameter μ becomes very small, the two typical solutions in (17) behave as $(1 - i\mu t)$ and $(1 + i\mu t)$, with the combination $(u_+ - u_-)/\mu$ limiting to a form that is linear in t.

[18] Since non-diagonalizable Hamiltonians can be constructed as limits of diagonalizable ones, the completeness of the eigenstates of a diagonalizable Hamiltonian translates into the completeness of the stationary plus non-stationary solutions to the non-diagonalizable one, with the counting being as given in [16].

[19] For a Hermitian Hamiltonian the time derivative of a probability such $\int d^3x\psi^*\psi$ can be written as an asymptotic surface term. This probability will be preserved in time if ψ is well-behaved at large distances. When a non-diagonalizable Hamiltonian is constructed as the limit of a diagonalizable one, there is modification in the behavior of ψ in time but not in space. Thus the asymptotic surface term continues to vanish, and $\int d^3x\psi^*\psi$ continues to be time-independent.